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Jose Rodriguez
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The symmetry of a single Cooper pair in a monolayer of hole-doped or electron-doped iron superconductor was determine at the limit of strong on-site Coulomb repulsion, with only the 3d xz and the 3d yz iron orbitals included. Exact numerical diagonalization that exploited AFRL supercomputers, in addition to meanfield theory, find isotropic pairing on the electron Fermi surface pockets plus isotropic pairing of opposite sign on hole bands buried below the Fermi level. These results potentially account for the hightemperature superconductivity displayed recently by surface layers of iron selenide.

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Final Report: Theoretical/Computational Studies of High-Temperature Superconductivity from Quantum Magnetism*

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Abstract

The symmetry of a single Cooper pair in a monolayer of hole-doped or electron-doped iron superconductor was determine at the limit of strong on-site Coulomb repulsion, with only the $3d_{xz}$ and the $3d_{yz}$ iron orbitals included. Exact numerical diagonalization that exploited AFRL supercomputers, in addition to meanfield theory, find isotropic pairing on the electron Fermi surface pockets plus isotropic pairing of opposite sign on hole bands buried below the Fermi level. These results potentially account for the high-temperature superconductivity displayed recently by surface layers of iron selenide.

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I. INTRODUCTION

Below, we describe the PI's scientific activity funded by AFSOR grant no. FA9550-13-1-0118. The funding period began March 1, 2013, and it ended February 29, 2016. The PI devoted this funding cycle to uncovering the symmetry of Cooper pairs in a single layer of iron-pnictide/selenide superconductor at the limit of strong on-site Coulomb repulsion. Exact diagonalization techniques that exploited DoD supercomputers at the AFRL were brought to bear on the difficult many-electron problem that the PI was faced with. This, in conjuction with a meanfield analysis, revealed a new groundstate for surface-layers FeSe that potentially accounts for the high-temperature superconductivity that these systems show.

II. PUBLICATIONS AND PRESENTATIONS

A. Publications

1. J.P. Rodriguez, M.A.N. Araujo, P.D. Sacramento, "Emergent Nesting of the Fermi Surface from Local-Moment Description of Iron-Pnictide High-Tc Superconductors", European Physical Journal B **87**, 163 (2014).

2. J.P. Rodriguez, "Collective Mode at Lifshitz Transition in Iron-Pnictide Superconductors", arXiv:1408.0864 , submitted to Journal of Physics: Condensed Matter.

3. J.P. Rodriguez, "Isotropic Cooper Pairs with Emergent Sign Changes in Single-Layer High-Tc Superconductors", arXiv:1601.01860, submitted to Physical Review Letters.

4. J.P. Rodriguez, "Particle-Hole Transformation in Iron-Based High-Temperature Superconductors", arXiv:1601.07479, submitted to Europhysics Letters.

B. Manuscripts in Preparation

1. J.P. Rodriguez and S. Haas, "High-Temperature Superconductivity in Surface-Layers of Iron Selenide: A Variational Monte Carlo Study".

2. J.P. Rodriguez, "High-Temperature Superconductivity versus Nematicity in Surface-Layers of Iron Selenide at the Strong Correlation Limit".

C. Presentations

1. J.P. Rodriguez, “Cooper Pair Formation from Quantum Magnetism in Iron-Pnictide High-Tc Superconductors” (contributed talk), 2013 March Meeting of the American Physical Society held in Baltimore, Maryland, March 18-22, 2013.

2. J.P. Rodriguez, “Iron-pnictide High-Tc Superconductivity from the limit of Local Magnetic Moments” (invited talk), Southern California Condensed Matter Theory Meeting held at California State University Long Beach, April 12, 2013.

3. J.P. Rodriguez, “Iron-Pnictide High-Tc Superconductivity from Local Magnetic Moments” (invited talk), 16th US-Japan Workshop on Advanced Superconductors, held at Dayton, Ohio, July 10-12, 2013.

4. J.P. Rodriguez, “Critical Current of Layered Superconductor with Columnar Defects in Tilted Magnetic Field: A Numerical Study” (contributed talk), 2014 March Meeting of the American Physical Society held in Denver, Colorado, March 3-7, 2014.

5. J.P. Rodriguez, “Collective Modes in Iron Superconductors from the Local Moment Limit” (invited talk), AFOSR Superconductivity Program Review 2014, held at the AFOSR, Arlington, Virginia, August 18, 2014.

6. J.P. Rodriguez, “Collective Modes in Iron Superconductors from the Local Moment Limit” (contributed talk), KITP Program on Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond, held at KITP, University of California Santa Barbara, September 2 - November 21, 2014.

7. J.P. Rodriguez, “Collective Modes in Iron Superconductors from the Local Moment Limit” (invited talk), Department of Physics and Astronomy, University of Southern California, February 27, 2015.

8. J.P. Rodriguez, “How to Exploit NUMA Computer Architecture on Lancer to Find New High-Tc Superconductors” (invited talk), 2015 Air Force High-Performance Computing User Forum, held at AFRL, Dayton, Ohio, July 20-24, 2015.

9. J.P. Rodriguez, “Are the New Class of Iron-Pnictide Superconductors Doped Mott Insulators?” (invited talk), Department of Physics and Astronomy, California State

University Northridge, September 30, 2015.

III. SCIENTIFIC VISITS

1. Invited to participate in the KITP Program on Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond, held at KITP, University of California Santa Barbara, September 2 - November 21, 2014.

2. Invited by Professor Stephan Haas for sabbatical visit at the Department of Physics and Astronomy, University of Southern California, April 1 - June 30, 2015.

IV. PRINCIPAL RESULT OF FUNDED RESEARCH

Recent experimental studies reveal high-temperature superconductivity in surface layers of iron selenide[1,2]. These include an FeSe mono-layer over various substrates[3–5], intercalated FeSe[6,7], and bulk FeSe dosed with alkali metals over the surface[8,9]. All of these systems share a common electronic structure: 2D electron Fermi surface pockets at the corners of the Brillouin zone. Unlike iron-pnictide superconductors, the 2D hole bands at the Brillouin zone center are buried entirely below the Fermi level. Furthermore, the critical temperatures in surface-layer FeSe superconductors lie inside the range $40 - 110$ K, which is substantially higher than the range of critical temperatures in iron-pnictide superconductors. All surface-layer FeSe superconductors also show an isotropic gap on the electron Fermi surface pockets[10]. The experimental findings listed above strongly suggest that the high-temperature superconductivity shown by surface-layer FeSe is due to a *new* underlying groundstate.

Calculations based on density-functional theory (DFT) typically predict hole Fermi surface pockets at the Brillouin zone center[11], which is counter to what is observed by angle-resolved photoemission (ARPES)[2,6,7,9,10]. The PI has recently shown that the buried hole bands shown at surface layers of FeSe can be understood instead as emergent phenomena. He includes only the $3d_{xz}$ and $3d_{yz}$ orbitals, along with strong on-site Coulomb repulsion. Proximity to hidden magnetic order yields electron Fermi surface pockets at the corners of the Brillouin zone and hole bands at the Brillouin zone center that lie entirely below the Fermi level[12].

The PI's theory also predicts isotropic Cooper-pair symmetry on the electron Fermi surface pockets, in addition to remnant isotropic Cooper pairing of opposite sign on the buried hole bands. This state of affairs occurs at a quantum-critical point tuned by Hund coupling, at which s-wave and d-wave Cooper pairs become degenerate in energy. Given the failure of DFT to describe electronic structure in surface layers of FeSe, the PI's approach based on emergent hole bands is possibly the only viable theory at the moment that describes the high-temperature superconductivity displayed by these new systems.

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Y.X. Wang, B.P. Xie, X.F. Lu, N.Z. Wang, X.H. Chen, Z. Sun, and D.L. Feng, "Surface electronic structure and isotropic superconducting gap in $(Li_{0.8}Fe_{0.2})OHFeSe$", Phys. Rev. B **92**, 060504(R) (2015).

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[11] T. Bazhirov and M.L. Cohen, "Effects of charge doping and constrained magnetization on the electronic structure of an FeSe monolayer", J. Phys.: Condens. Matter **25**, 105506 (2013).

[12] J.P. Rodriguez, "Isotropic Cooper Pairs with Emergent Sign Changes in Single-Layer High-Tc Superconductors", arXiv:1601.01860, submitted to Physical Review Letters.

1.

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Jose P. Rodriguez

Program Manager

The AFOSR Program Manager currently assigned to the award

Dr. Harold Weinstock

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The symmetry of a single Cooper pair in a monolayer of hole-doped or electron-doped iron superconductor was determine at the limit of strong on-site Coulomb repulsion, with only the 3d xz and the 3d yz iron orbitals included. Exact numerical diagonalization that exploited AFRL supercomputers, in addition to meanfield theory, find isotropic pairing on the electron Fermi surface pockets plus isotropic pairing of opposite sign on hole bands buried below the Fermi level. These results potentially account for the high-temperature superconductivity displayed recently by surface layers of iron selenide.

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Archival Publications (published) during reporting period:

1. J.P. Rodriguez, M.A.N. Araujo, P.D. Sacramento, "Emergent Nesting of the Fermi Surface from Local-Moment Description of Iron-Pnictide High-Tc Superconductors", European Physical Journal B 87, 163 (2014).

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